MAR 19 1965

United States Army
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Philadelphia, Pa., 19137

ADDRESS REPLY TO
COMMANDING OFFICER
FRANKFORD ARSENAL
ATTN: SMUFA - 1312 (L6200)
S. H. EISMAN

15 March 1965

Prof. Joshua Lederberg
Department of Genetics
Stanford University
Medical Center
Palo Alto, California

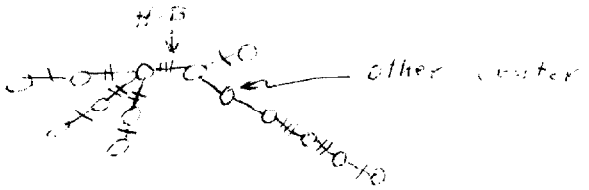
Dear Prof. Lederberg:

Thank you very much for the updated version of DENDRAL.

Is the algorithm for determining the Henze-Blair center of a tree relatively simple and fast, or is it necessary to enumerate numbers of nodes connected to each bond and then make comparisons? An algorithm for determining the center of a tree as defined by Berge or Ore (that node or pair of nodes, n, for which max d(n,x) is a minimum where x ranges over all other nodes and d(n,x) is the number of links between n and x) with which I am familiar is:

1. Label all end nodes and their adjacent links
2. Remove all labelled nodes and links
3. If more than two nodes are left, return to 1. Otherwise, the remainder is the 'center'.

e.g.



I agree that the method of H and B using their notion of the central atom is quite useful for systematically generating isomers, possible the only way. But I don't see a simple or short way of systematically finding the H B center for a given tree even though I know that the number of nodes must satisfy restricted partitions of n-1.

You may be interested to know that Gluck's paper appeared in J. Chem. Documentation V. 5, #1, Feb. '65, pp 43-51. If you look at his 'compact list' on page 47 you'll notice the similarity with the Polish Dendral ideas. His column labelled 'Atom to list' is superfluous if a little care is taken. The only difference is that instead of going to all descendants of a node in order, he lists by specific order within each generation. This is an equivalent tree naming system and algorithms exist for transforming between it and the 'descendant' ordered notation.

Sincerely yours,

S. H. EISMAN